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# **Level-2 Milestone 4468:** ***Lorenz Simulation Interface*** ***Beta Release***

**Milestone Report for NNSA HQ**

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*December 21, 2011*

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# Introduction

This report documents LLNL Lorenz project activities related to simulation web interfaces, ASC L2 milestone NNN: Lorenz Simulation Interface Beta Release, due December 31, 2011. The full text of the milestone is included in Attachment 1. The description of milestone is:

*This milestone builds upon the Lorenz HPC job management application, a web-based tool for submitting and managing batch jobs. FY12 work will encompass the following new Lorenz deliverables: 1) a web-based interface for specifying and launching a vertical application of interest to ASC, and 2) the associated web service infrastructure for supporting these operations. The Lorenz project is focused on making HPC easier and more efficient through the use of state-of-the-art web technologies..*

The milestone was completed on December 21, 2011 when a fully functional web interface to pre-defined ParaDiS simulations was made available to beta users. Gregg Hommes from the ParaDiS team successfully specified, customized, and submitted a ParaDiS simulation on an LC system through the Lorenz web interface.

A letter certifying that the ParaDiS code team verified correct and complete operation of the Lorenz simulation interface is included as Attachment 2. An overview of the Lorenz system architecture is included as Attachment 3. Screen captures of the Lorenz simulation interface are provided in Attachment 4.

# Lorenz Project Overview

The goal of Lorenz is to develop a sophisticated web-based framework as a front end to Livermore Computing Center resources. The primary features include: a personalized dashboard for each user, giving an at-a-glance overview of all computing center resources; a front-end to job submission and management; and a software framework to extend the convenience of web interfaces into simulation codes, including support for setting up, launching, steering, and monitoring simulations.

Because the breadth of desktop operating systems in use both inside and outside LLNL spans all flavors of Linux, Mac, and Windows, the decision was made to use exclusively web-based technologies in Lorenz. Recent advancements in AJAX and Javascript programming, along with coming advances in the form of HTML5 and CSS3, made the browser the preferred development platform. The goal is to provide the user with a robust application interface that requires nothing more than a modern, standards-based web browser. This approach not only provides convenient access to Lorenz for internal and external users, but also has significant advantages over conventional applications in terms of rapid deployment and updates.

The first phase of the Lorenz project is a system “dashboard”, known as MyLC, that gives LC users a rich set of portal applications, or “portlets”, from which to choose. Information that previously required knowledge of dozens of different commands, files, and web pages is now available in one convenient location. This includes account information, bank and disk usage, quotas, cluster utilization, news items, active jobs on LC systems, and more. The extensible software design of the dashboard allows users and staff members to develop their own portlets, and for them to be shared with all users or just within work groups.

The second major phase of Lorenz was built on the idea that HPC centers are managed around batch processing, and “jobs” (or “runs”) progress through several discrete stages: setup, submission, queuing/waiting, running, completion, analysis, and archiving. Lorenz aims to ultimately tie all of these pieces together, including integration with the dashboard and application portals. In addition to helping guide users through the process of defining batch parameters, monitoring job progress, and interacting with jobs and job output, Lorenz also aims to promote access to additional tools and capabilities which to this point have been limited to use by power users. Ultimately Lorenz will assist users in choosing the appropriate resources, such as cluster and file system, given the requirements of a job.

The third major phase of Lorenz, the subject of this milestone, is the development of an application portal. This involves teaming with application codes to provide a simple graphical interface to the simulations, which in turn seamlessly ties into job submission and monitoring. This will allow users to directly define simulation parameters and launch applications using a simple but powerful web front-end.

Because many complex multi-physics codes can have thousands of inputs, providing a general GUI for building an input deck from scratch is impractical. However, most users of large applications start with an existing input file, and make some number of small changes to it. The application portal will feature a process that combines trusted and

validated input files with a GUI that guides the user toward making the relatively minor changes needed for their particular problem. The input files will be in the form of templates, containing most of the data needed for a particular problem along with parameterization of changeable inputs. For expert users, there ultimately will be a way to edit the final input file directly - in the event that there are input changes needed that were not captured in the GUI.

## Attachment 1: Milestone Definition Text

<b>Milestone (4468): Lorenz Simulation Interface Beta Release</b>		
<b>Level:</b> 2	<b>Fiscal Year:</b> FY12	<b>DOE Area/Campaign:</b> ASC
<b>Completion Date:</b> 12/31/11		
<b>ASC nWBS Subprogram:</b> CSSE		
<b>Participating Sites:</b> LLNL		
<b>Participating Programs/Campaigns:</b> ASC		
<b>Description:</b> This milestone builds upon the Lorenz job management application, a Web-based tool for submitting and managing batch jobs. FY12 work will encompass the following new Lorenz deliverables: 1) a Web-based interface for specifying and launching a vertical application of interest to ASC, and 2) the associated Web service infrastructure for supporting these operations. The Lorenz project is focused on making HPC easier and more efficient through the use of state-of-the-art Web technologies.		
<b>Completion Criteria:</b> This milestone is complete when users are able to use the Lorenz Web application to populate a simulation input deck, as well as launch and monitor jobs on both the classified and unclassified networks at LLNL.		
<b>Customer:</b> SSP and weapons science customers.		
<b>Milestone Certification Method:</b> Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion. The “handoff” of the developed capability (product) to a nuclear weapons stockpile customer is documented.		
<b>Supporting Resources:</b> LC Division personnel and ASC customers.		
<b>Supporting Milestones:</b>		
<b>Program</b>	<b>Title</b>	<b>Due Date</b>
N/A		
<b>Codes/Simulation Tools Employed:</b> None		
<b>Contribution to the ASC Program:</b> Improved ability to manage, monitor, and launch simulation jobs running on ASC supercomputers.		
<b>Contribution to Stockpile Stewardship:</b> Improved ability to manage, monitor, and launch simulation jobs running on ASC supercomputers.		

<b>Milestone (4468): Lorenz Simulation Interface Beta Release</b>				
<b>No.</b>	<b>Risk Description</b>	<b>Risk Assessment (low, medium, high)</b>		
		<b>Consequence</b>	<b>Likelihood</b>	<b>Exposure</b>
1.	Schedule slips	Low	Low	Low



## **Attachment 2: Handoff Letter**



December 22, 2011

To: Michel McCoy, LLNL ASC Program Leader  
From: Gregg Hommes  
Subject: Completion of ASC Level 2 Milestone 4468

I certify that the Lorenz simulation interface for the ParaDiS application has been made available as a beta release. Multiple pre-defined simulation options are available to users, including copper and tantalum. Using the Lorenz web interface, simulation input parameters of interest to users can be modified, and jobs can easily be submitted to LC HPC resources.

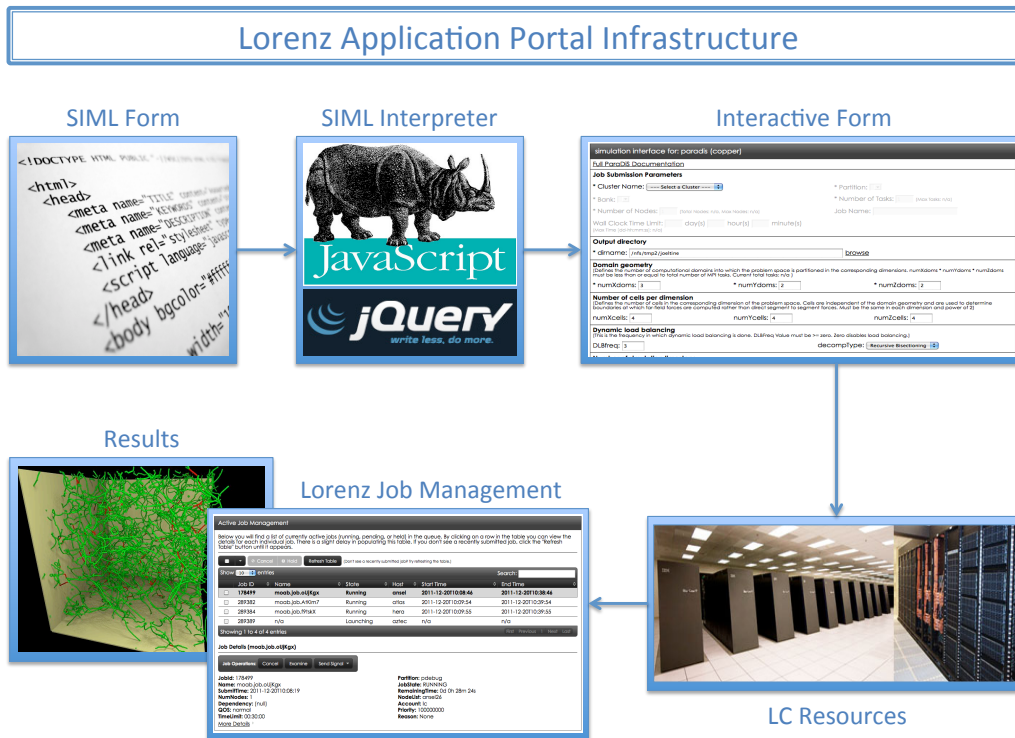
The beta release of the Lorenz simulation interface capability meets the milestone completion criteria for L2 Milestone 4468, Lorenz Simulation Interface Beta Release.

A handwritten signature in blue ink, reading "Gregg Hommes", is positioned above a horizontal line.

Gregg Hommes  
ParaDiS Code Developer



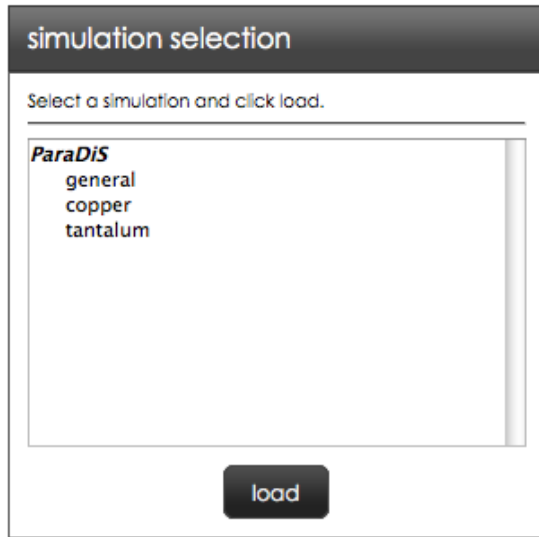
# Attachment 3: The Lorenz Application Portal Architecture



## Lorenz System Architecture for the Application Portal

The Lorenz application portal makes use of forms written in the Simulation Input Markup Language (SIML). These forms are interpreted into HTML format and presented in the user's web browser. After completing and submitting the form, simulation input files are created on an LC resource, and a batch job is submitted. The user is directed to the Lorenz job management element to monitor progress, as well as to examine the results of the completed simulation.

## Attachment 4: Lorenz Screenshots



Screen capture of the simulation selector, part of the Lorenz Application Portal.

simulation select >> paradis (copper)

simulation interface for: paradis (copper)

Job Submission Parameters

\* Cluster Name:

\* Bank:

\* Number of Nodes:  (Total Nodes: 296, Max Nodes: 296)

Wall Clock Time Limit:  day(s)  hour(s)  minute(s)  
(Max Time [dd-hh:mm:ss]: 12:00:00)

\* Partition:

\* Number of Tasks:  (Max Tasks: 12)

Job Name:

Output directory

\* dirname:

[browse](#)

Domain geometry

(Defines the number of computational domains into which the problem space is partitioned in the corresponding dimensions. numXdoms \* numYdoms \* numZdoms must be less than or equal to total number of MPI tasks. Current total tasks: 12)

\* numXdoms:

\* numYdoms:

\* numZdoms:

Number of cells per dimension

(Defines the number of cells in the corresponding dimension of the problem space. Cells are independent of the domain geometry and are used to determine boundaries at which far-field forces are computed rather than direct segment to segment forces. Must be the same in each dimension and power of 2)

numXcells:

numYcells:

numZcells:

Dynamic load balancing

(This is the frequency in which dynamic load balancing is done. DLBFreq Value must be >= zero. Zero disables load balancing.)

DLBFreq:

decompType:

Number of simulation timesteps

maxstep:

Discretization and topological change controls

(MaxSeg Value must be such that no dislocation can span a full FMM cell which, ties it to the num{XYZ}cells parameters above and to the actual simulation size defined in the nodal data file. Must be less than: 450)

\* maxSeg:

enableCrossSlip: ☒

enforceGlidePlanes: ☒

Load type

(Defines the type of load applied to the system)

loadType:

?

Sets the maximum permitted length of a dislocation segment. Primarily used for determining when segments are to be rediscrtized during remesh operations. This value must be < 9/10 the cell size of a cell.

Screen capture of Lorenz simulation interface for ParaDiS, with copper option.

enableCrossSlip: ☒ ?

**Load type**  
(Defines the type of load applied to the system)  
loadType: constant strain rate

**Mobility module**  
mobilityLaw: FCC\_0

**Core radius for self-force calcs**  
\* rc: 5.0 ?

**Output Parameters**

**Flux decomposition files**  
fluxfile: ☒ ?

**Gnuplot files**  
gnuplot: ☒ ?

**Restart files**  
savecn: ☒ ? savecnfreq: 500

**Various properties files**  
saveprop: ☒ ? savepropfreq: 100

**Node and or segment data files for use with Visit**  
writeVisit: ☒ ? writeVisitFreq: 200  
writeVisitBurgID: ☒ ?

Run Simulation

**Simulation Submit Successful**

Your simulation has been successfully submitted! Click the "Go To Job Management" button below to track your job through the job management interface.

Go To Job Management OK

Screen capture of Lorenz response after submitting simulation.

**Active Job Management**

Below you will find a list of currently active jobs (running, pending, or held) in the queue. By clicking on a row in the table you can view the details for each individual job. There is a slight delay in populating this table. If you don't see a recently submitted job, click the "Refresh Table" button until it appears.

Refresh Table button available in 5 (Don't see a recently submitted job? Try refreshing the table.)

Show 10 entries Search:

Job ID	Name	State	Host	Start Time	End Time
178297	Paradis_ansel	Pending	ansel	N/A	N/A

Showing 1 to 1 of 1 entries First Previous 1 Next Last

**Job Details (Paradis\_ansel)**

**JobId:** 178297  
**Name:** Paradis\_ansel  
**SubmitTime:** 2011-12-19T10:19:23:00  
**NumNodes:** 1  
**Dependency:**  
**QOS:** normal  
**TimeLimit:** 8:00:00  
[More Details](#)

**Partition:** pbatch  
**JobState:** JobHeldSystem  
**RemainingTime:**  
**NodeList:**  
**Account:** lc  
**Priority:**  
**Reason:**

Screen capture of Lorenz job management page showing job submitted via the Application Portal